SPORES
Structure PrOtonation and REcognition System
user manual for academic trial version

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1 running SPORES

In this trial version of the structure recognition and protonation tool SPORES five running-modes are implemented: complete protonation and reprotonation for mol2 and pdb files and adjustment of Sybyl-Types for atoms and bonds without altering the protonation for mol2 files only. SPORES can be executed by typing *SPORES - -mode running-mode yourinputfile youroutputfile* where *running-mode* is one of the options below. *yourinputfile* is the structure file used as input in pdb or mol2 format. *youroutputfile* is the protonated structure file of your molecule in mol2 format.

1.1 running-modes for pdb input files

For processing pdb files SPORES need files from the remediated data base due to its reading routine. The output will be written in mol2 format.

- **completepdb**: structure recognition and protonation
- **reprotpdb**: deletes all hydrogen atoms from a pdb file and reprotonates the input structure

1.2 running-modes for mol2 input files

- **completemol2**: structure recognition and protonation
- **reprot**: deletes all hydrogen atoms and reprotonates the input structure
- **settypes**: for protonated structures, checks connectivity and assigns Sybyl atom and bond types

2 SPORES full version

The full version of SPORES includes additional running modes for generation of protonation states, tautomers and stereoisomers along with other features like retaining all bond types but readjusting the atom types.